wwPDB EM Validation Summary Report (i)

May 4, 2024 – 04:14 PM EDT

PDB ID	:	8T0E
EMDB ID	:	EMD-40941
Title	:	TRPV1 in Nanodisc not bound with lysophosphatidic acid (apo)
Authors	:	Arnold, W.R.; Cheng, Y.
Deposited on	:	2023-05-31
Resolution	:	3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

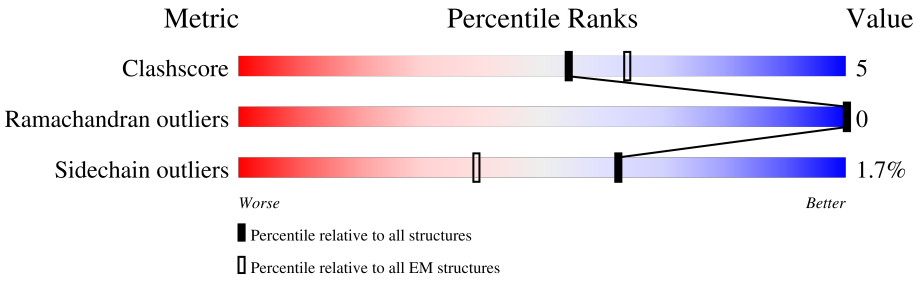
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	815	56% 9% 35%
1	B	815	55% 9% 35%
1	C	815	56% 9% 35%
1	D	815	56% 9% 35%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 35093 atoms, of which 17660 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	531	Total	C	H	N	O	S	0	0
			8669	2826	4357	699	762	25		
1	D	531	Total	C	H	N	O	S	0	0
			8669	2826	4357	699	762	25		
1	B	531	Total	C	H	N	O	S	0	0
			8669	2826	4357	699	762	25		
1	C	531	Total	C	H	N	O	S	0	0
			8669	2826	4357	699	762	25		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP O35433
A	?	-	ASN	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	LEU	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	MET	deletion	UNP O35433
A	?	-	GLU	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	THR	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	HIS	deletion	UNP O35433
A	?	-	LYS	deletion	UNP O35433
A	?	-	CYS	deletion	UNP O35433
A	?	-	ARG	deletion	UNP O35433
A	?	-	GLY	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
A	?	-	ALA	deletion	UNP O35433
A	?	-	CYS	deletion	UNP O35433
A	?	-	LYS	deletion	UNP O35433
A	?	-	PRO	deletion	UNP O35433
A	?	-	GLY	deletion	UNP O35433

Continued on next page...

Continued from previous page...

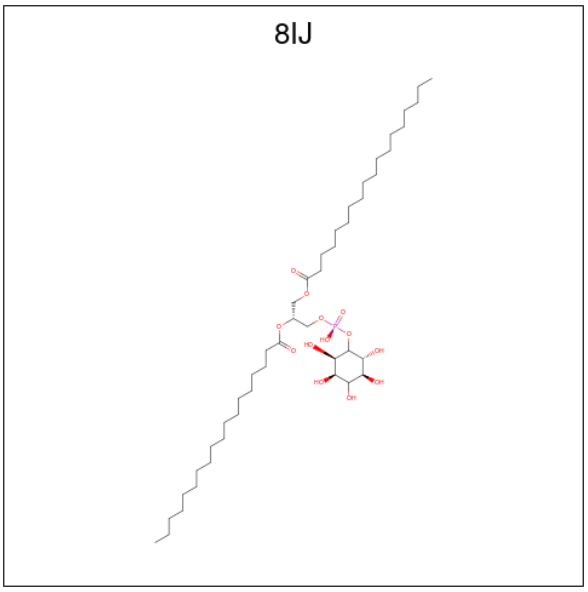
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP O35433
A	?	-	SER	deletion	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	LEU	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	MET	deletion	UNP O35433
D	?	-	GLU	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	THR	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	HIS	deletion	UNP O35433
D	?	-	LYS	deletion	UNP O35433
D	?	-	CYS	deletion	UNP O35433
D	?	-	ARG	deletion	UNP O35433
D	?	-	GLY	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
D	?	-	ALA	deletion	UNP O35433
D	?	-	CYS	deletion	UNP O35433
D	?	-	LYS	deletion	UNP O35433
D	?	-	PRO	deletion	UNP O35433
D	?	-	GLY	deletion	UNP O35433
D	?	-	ASN	deletion	UNP O35433
D	?	-	SER	deletion	UNP O35433
B	?	-	ASN	deletion	UNP O35433
B	?	-	ASN	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
B	?	-	LEU	deletion	UNP O35433
B	?	-	PRO	deletion	UNP O35433
B	?	-	MET	deletion	UNP O35433
B	?	-	GLU	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
B	?	-	THR	deletion	UNP O35433
B	?	-	PRO	deletion	UNP O35433
B	?	-	HIS	deletion	UNP O35433
B	?	-	LYS	deletion	UNP O35433
B	?	-	CYS	deletion	UNP O35433
B	?	-	ARG	deletion	UNP O35433
B	?	-	GLY	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
B	?	-	ALA	deletion	UNP O35433

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	CYS	deletion	UNP O35433
B	?	-	LYS	deletion	UNP O35433
B	?	-	PRO	deletion	UNP O35433
B	?	-	GLY	deletion	UNP O35433
B	?	-	ASN	deletion	UNP O35433
B	?	-	SER	deletion	UNP O35433
C	?	-	ASN	deletion	UNP O35433
C	?	-	ASN	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433
C	?	-	LEU	deletion	UNP O35433
C	?	-	PRO	deletion	UNP O35433
C	?	-	MET	deletion	UNP O35433
C	?	-	GLU	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433
C	?	-	THR	deletion	UNP O35433
C	?	-	PRO	deletion	UNP O35433
C	?	-	HIS	deletion	UNP O35433
C	?	-	LYS	deletion	UNP O35433
C	?	-	CYS	deletion	UNP O35433
C	?	-	ARG	deletion	UNP O35433
C	?	-	GLY	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433
C	?	-	ALA	deletion	UNP O35433
C	?	-	CYS	deletion	UNP O35433
C	?	-	LYS	deletion	UNP O35433
C	?	-	PRO	deletion	UNP O35433
C	?	-	GLY	deletion	UNP O35433
C	?	-	ASN	deletion	UNP O35433
C	?	-	SER	deletion	UNP O35433

- Molecule 2 is (2R)-3-{[(R)-hydroxy{[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dioctadecanoate (three-letter code: 8IJ) (formula: $C_{45}H_{87}O_{13}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	O	P	0
			101	31	56	13	1	
2	D	1	Total	C	H	O	P	0
			101	31	56	13	1	
2	B	1	Total	C	H	O	P	0
			101	31	56	13	1	
2	C	1	Total	C	H	O	P	0
			101	31	56	13	1	

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Na	0
			1	1	

- Molecule 4 is water.

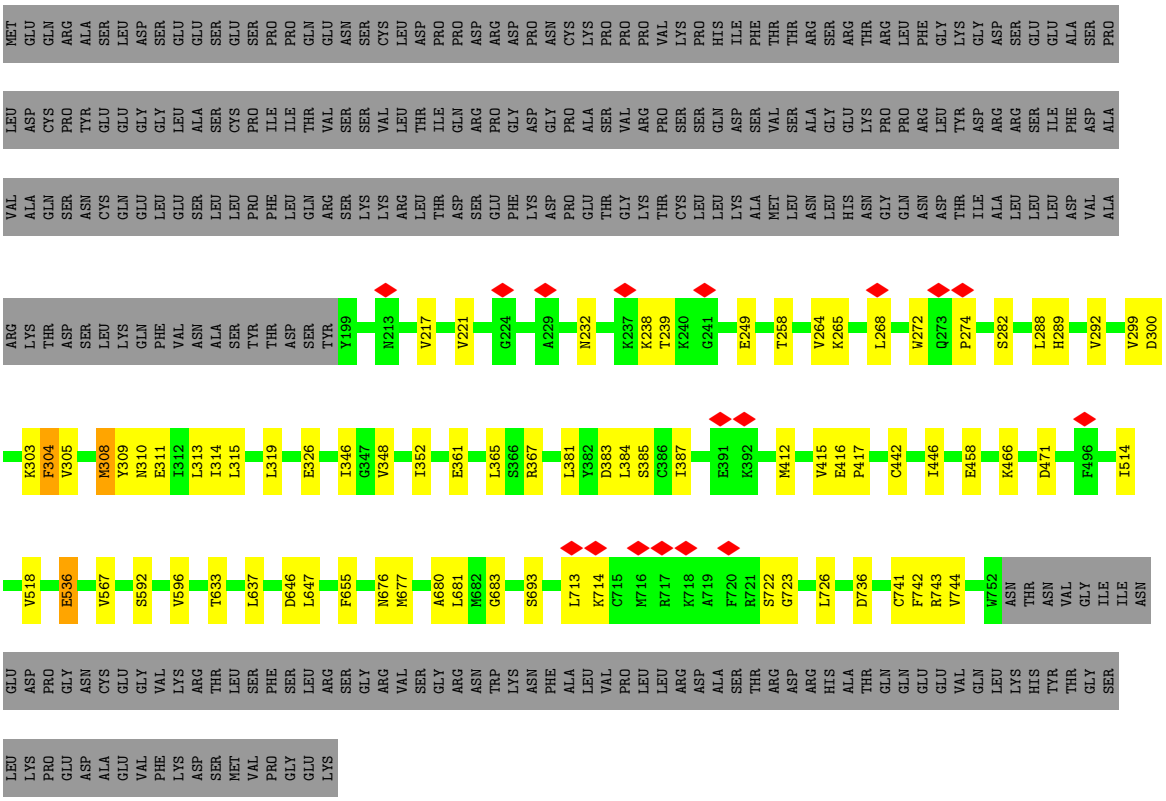
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	H	O	0
			3	2	1	
4	D	1	Total	H	O	0
			3	2	1	
4	B	1	Total	H	O	0
			3	2	1	
4	C	1	Total	H	O	0
			3	2	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

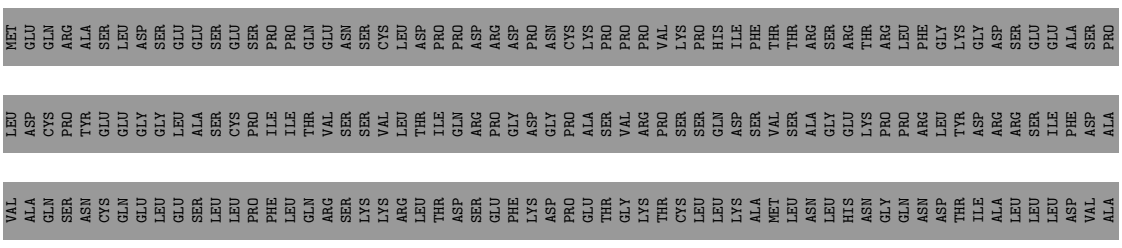
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

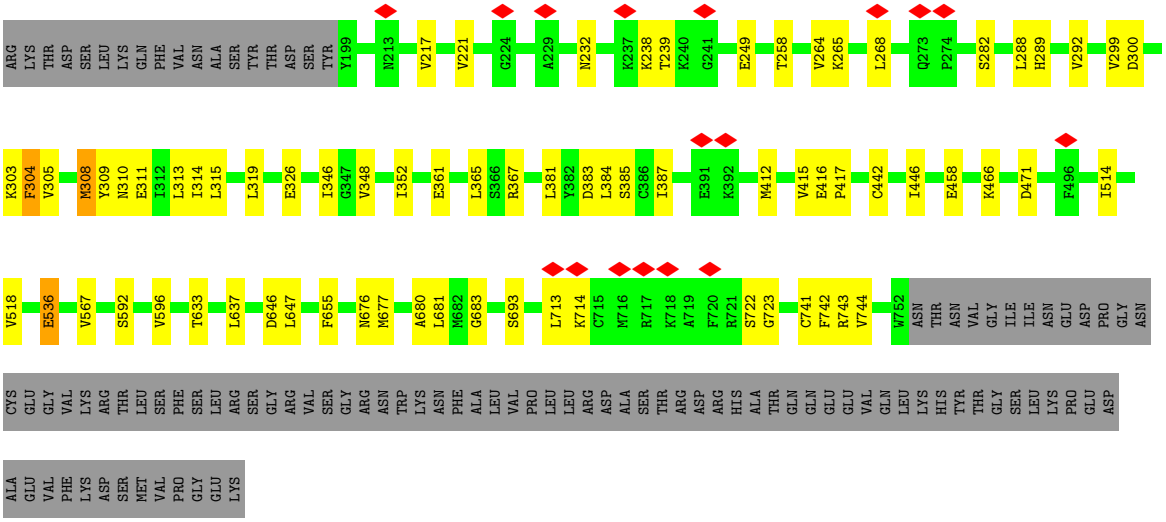
Chain A:



• Molecule 1: Transient receptor potential cation channel subfamily V member 1

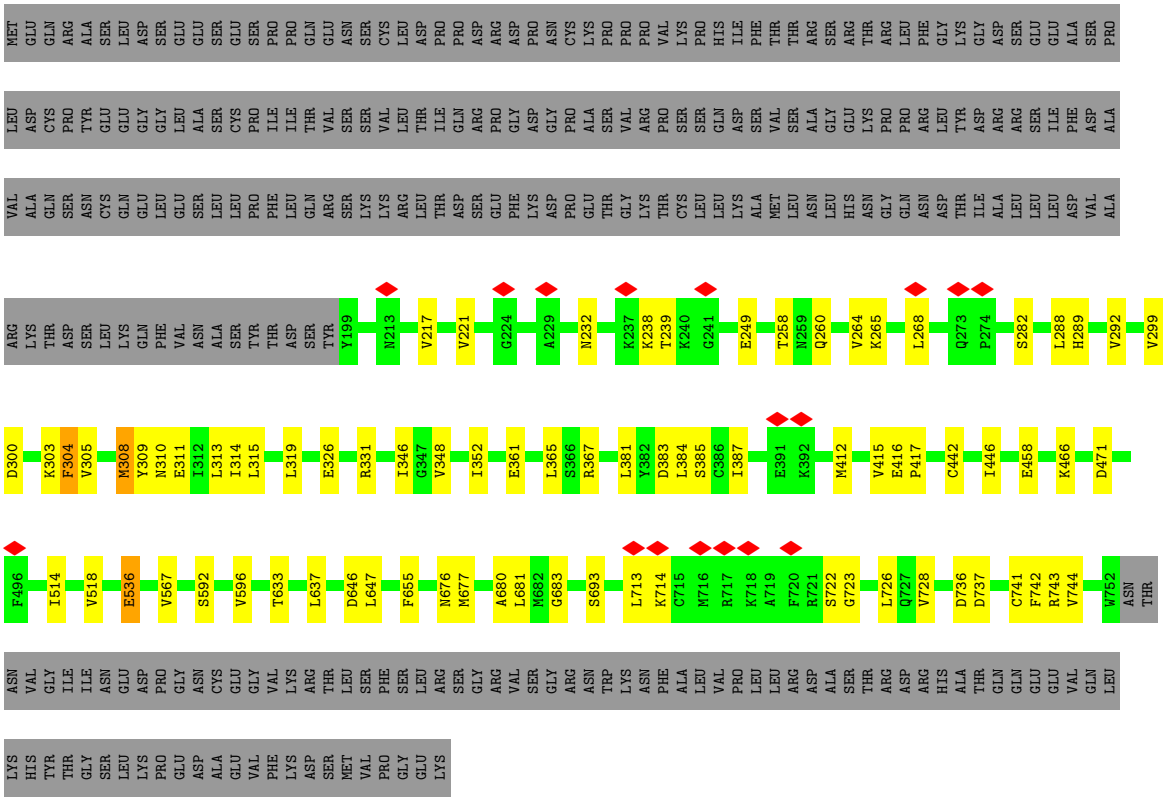
Chain D:





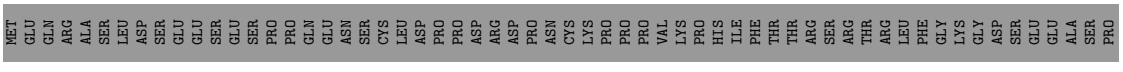
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

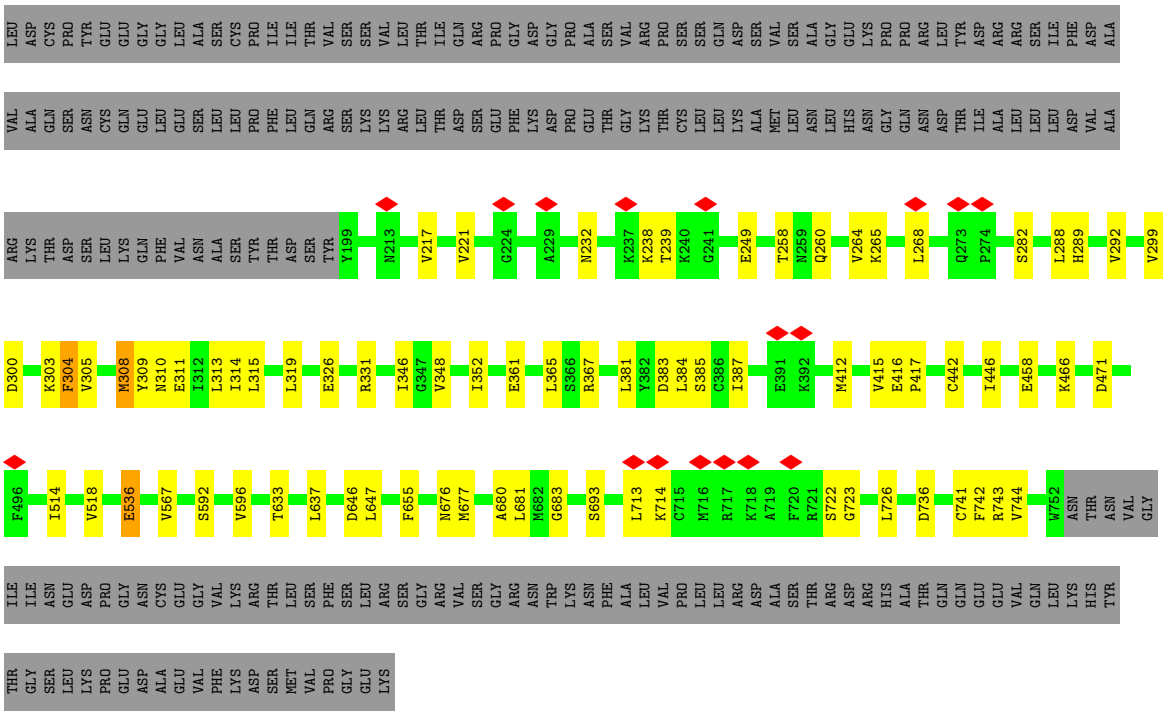
Chain B:



• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain C:




LEU ASP CYS PRO TYR GLU GLU GLY GLY LEU ALA SER CYS PRO ILE ILE THR VAL SER SER VAL LEU THR ILE GLN ARG PRO GLY ASP GLY PRO ALA SER VAL ARG PRO SER SER GLN ASP SER VAL SER ALA GLY GLU LYS PRO PRO ARG LEU TYR ASP ARG ARG SER ILE PHE ASP ALA
VAL ALA GLN SER ASN CYS GLN GLU LEU GLU SER LEU LEU PRO PHE LEU GLN ARG SER LYS LYS ARG LEU THR ASP SER GLU PHE LYS ASP PRO GLU THR GLY LYS THR CYS LEU LEU LYS ALA MET LEU ASN LEU HIS ASN GLY GLN ASN ASP THR ILE ALA LEU LEU LEU ASP VAL ALA
ARG LYS THR ASP SER LEU LYS GLN PHE VAL ASN ALA SER TYR THR ASP SER TYR Y199 N213 V217 V221 G224 A229 N232 K237 K238 T239 K240 G241 E249 T258 N259 Q260 V264 K265 L268 Q273 P274 S282 L288 H289 V292 V299
D300 K303 F304 V305 M308 Y309 N310 E311 I312 L313 I314 L315 L319 E326 R331 I346 G347 V348 I352 E361 L365 S366 R367 L381 Y382 D383 L384 S385 C386 I387 E391 K392 M412 V415 E416 P417 C442 I446 E458 K466 D471
F496 I514 V518 E536 V567 S592 V596 T633 L637 D646 L647 F655 N676 M677 A680 L681 M682 G683 S693 L713 K714 C715 M716 R717 K718 A719 F720 R721 S722 G723 L726 D736 C741 F742 R743 V744 W752 ASN THR ASN VAL GLY
ILE ILE ASN GLU ASP PRO GLY ASN CYS GLU GLY VAL LYS ARG THR LEU SER PHE SER LEU ARG SER GLY ARG VAL SER GLY ARG ASN TRP LYS ASN PHE ALA LEU VAL PRO LEU LEU ARG ASP ALA SER THR ARG ASP ARG HIS ALA THR GLN GLN GLU GLU VAL GLN LEU LYS HIS TYR
THR GLY SER LEU LYS PRO GLU ASP ALA GLU VAL PHE LYS ASP SER MET VAL PRO GLY GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	4090	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	37.482	Depositor
Minimum map value	-27.390	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	320.63998, 320.63998, 320.63998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 8IJ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.37	1/4416 (0.0%)	0.55	2/5979 (0.0%)
1	B	0.37	1/4416 (0.0%)	0.55	2/5979 (0.0%)
1	C	0.37	1/4416 (0.0%)	0.55	2/5979 (0.0%)
1	D	0.37	1/4416 (0.0%)	0.55	2/5979 (0.0%)
All	All	0.37	4/17664 (0.0%)	0.55	8/23916 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	GLU	CD-OE2	-6.73	1.18	1.25
1	D	249	GLU	CD-OE2	-6.73	1.18	1.25
1	B	249	GLU	CD-OE2	-6.73	1.18	1.25
1	C	249	GLU	CD-OE2	-6.73	1.18	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	249	GLU	CB-CG-CD	-5.79	98.56	114.20
1	D	249	GLU	CB-CG-CD	-5.79	98.56	114.20
1	B	249	GLU	CB-CG-CD	-5.79	98.56	114.20
1	C	249	GLU	CB-CG-CD	-5.79	98.56	114.20
1	A	676	ASN	CB-CA-C	5.15	120.69	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4312	4357	4356	52	0
1	B	4312	4357	4356	54	0
1	C	4312	4357	4356	51	0
1	D	4312	4357	4356	48	0
2	A	45	56	0	1	0
2	B	45	56	0	1	0
2	C	45	56	0	0	0
2	D	45	56	0	0	0
3	A	1	0	0	0	0
4	A	1	2	0	0	0
4	B	1	2	0	0	0
4	C	1	2	0	0	0
4	D	1	2	0	0	0
All	All	17433	17660	17424	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 187 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:GLU:HG3	1:C:655:PHE:CZ	2.26	0.71
1:A:655:PHE:CZ	1:B:536:GLU:HG3	2.26	0.70
1:B:655:PHE:CZ	1:C:536:GLU:HG3	2.26	0.70
1:A:536:GLU:HG3	1:D:655:PHE:CZ	2.25	0.69
1:C:310:ASN:O	1:C:314:ILE:HD12	1.94	0.68

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	529/815 (65%)	474 (90%)	55 (10%)	0	100	100
1	B	529/815 (65%)	474 (90%)	55 (10%)	0	100	100
1	C	529/815 (65%)	474 (90%)	55 (10%)	0	100	100
1	D	529/815 (65%)	474 (90%)	55 (10%)	0	100	100
All	All	2116/3260 (65%)	1896 (90%)	220 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	469/722 (65%)	461 (98%)	8 (2%)	60	78
1	B	469/722 (65%)	461 (98%)	8 (2%)	60	78
1	C	469/722 (65%)	461 (98%)	8 (2%)	60	78
1	D	469/722 (65%)	461 (98%)	8 (2%)	60	78
All	All	1876/2888 (65%)	1844 (98%)	32 (2%)	62	78

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	308	MET
1	C	326	GLU
1	D	308	MET
1	D	304	PHE
1	C	536	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	8IJ	D	901	-	45,45,59	1.15	3 (6%)	55,57,71	1.25	6 (10%)
2	8IJ	A	901	-	45,45,59	1.15	3 (6%)	55,57,71	1.25	6 (10%)
2	8IJ	B	901	-	45,45,59	1.15	3 (6%)	55,57,71	1.25	6 (10%)
2	8IJ	C	901	-	45,45,59	1.14	3 (6%)	55,57,71	1.25	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8IJ	D	901	-	-	20/40/64/78	0/1/1/1
2	8IJ	A	901	-	-	20/40/64/78	0/1/1/1
2	8IJ	B	901	-	-	20/40/64/78	0/1/1/1
2	8IJ	C	901	-	-	20/40/64/78	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	8IJ	O40-C18	-3.05	1.39	1.46
2	D	901	8IJ	O40-C18	-3.04	1.39	1.46
2	A	901	8IJ	O40-C18	-3.01	1.39	1.46
2	C	901	8IJ	O40-C18	-3.01	1.39	1.46
2	B	901	8IJ	O20-C19	-2.74	1.38	1.45

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	8IJ	O40-C41-C43	3.84	119.78	111.50
2	B	901	8IJ	O40-C41-C43	3.84	119.78	111.50
2	C	901	8IJ	O40-C41-C43	3.81	119.72	111.50
2	A	901	8IJ	O40-C41-C43	3.81	119.72	111.50
2	B	901	8IJ	O20-C21-C23	2.90	121.01	111.91

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	8IJ	C14-C5-O4-P2
2	A	901	8IJ	C17-O16-P2-O1
2	A	901	8IJ	C17-O16-P2-O3
2	D	901	8IJ	C14-C5-O4-P2
2	D	901	8IJ	C17-O16-P2-O1

There are no ring outliers.

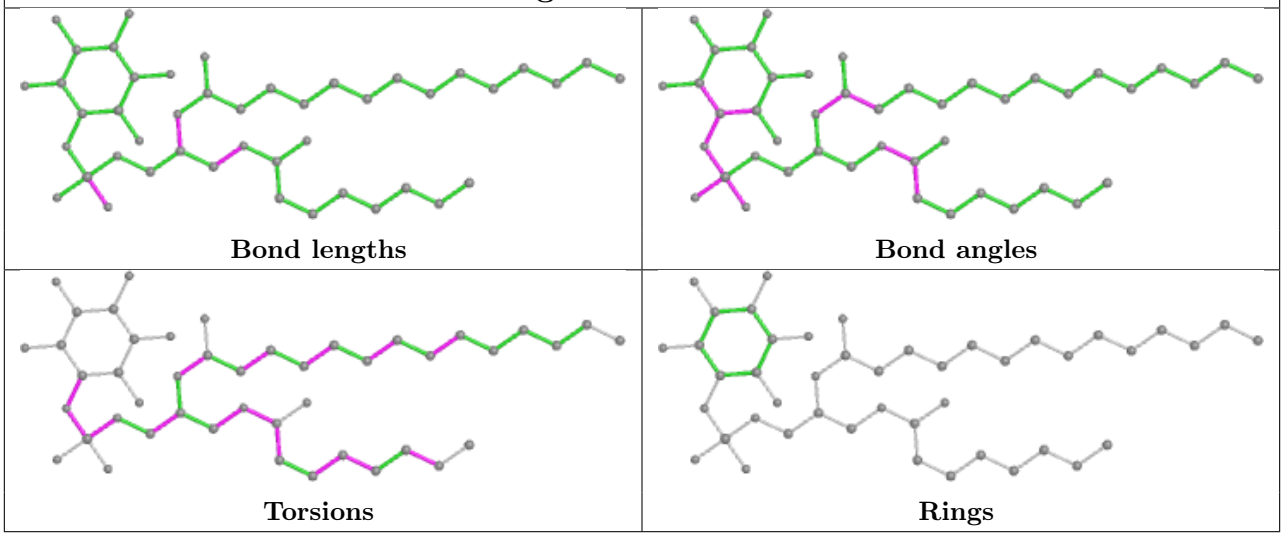
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	8IJ	1	0
2	B	901	8IJ	1	0

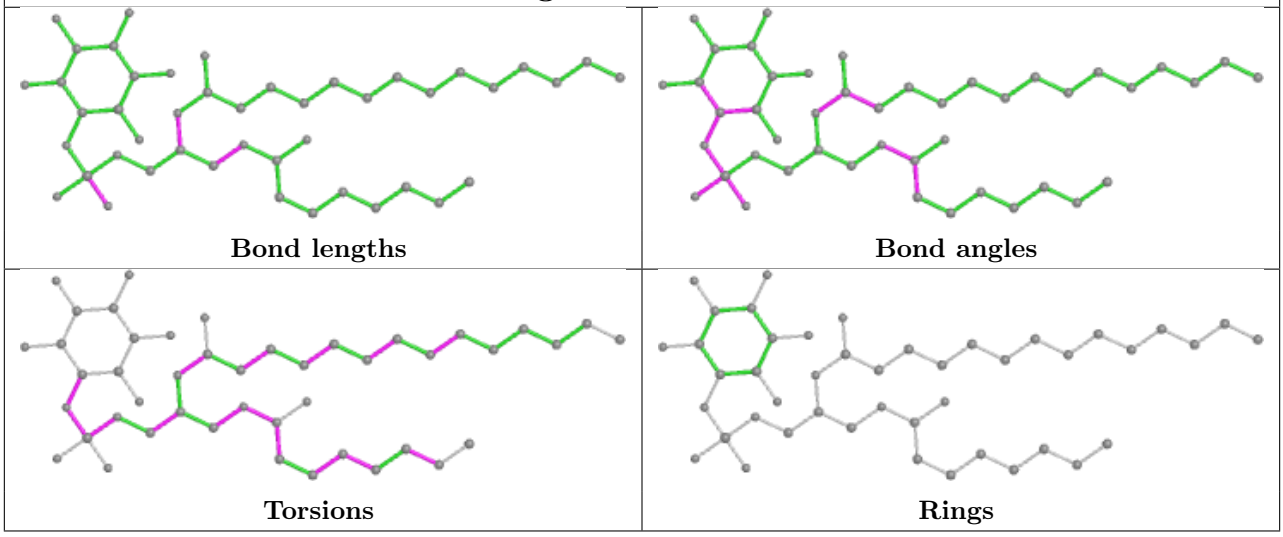
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

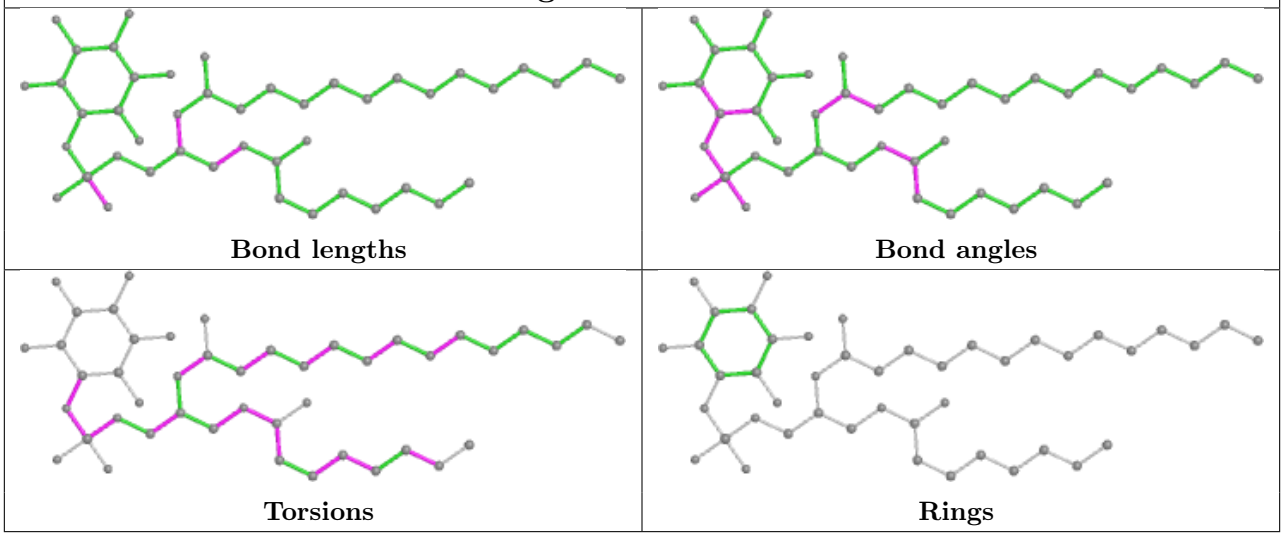
Ligand 8IJ D 901



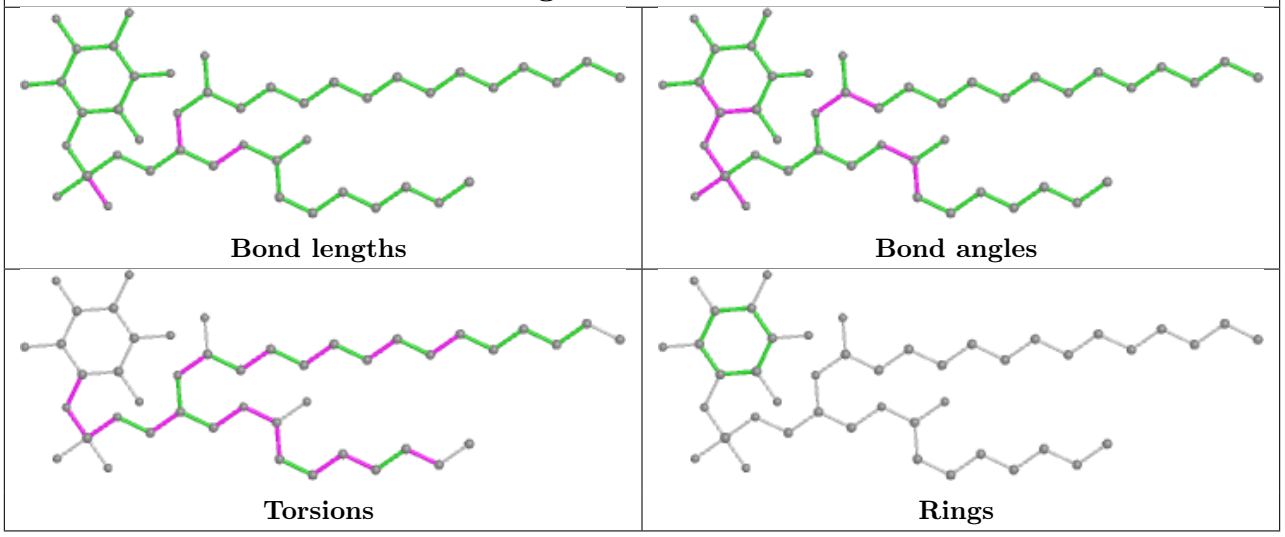
Ligand 8IJ A 901



Ligand 8IJ B 901



Ligand 8IJ C 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

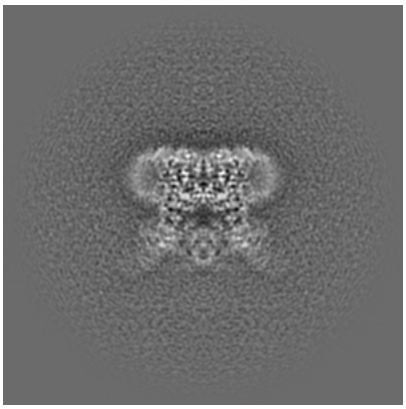
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40941. These allow visual inspection of the internal detail of the map and identification of artifacts.

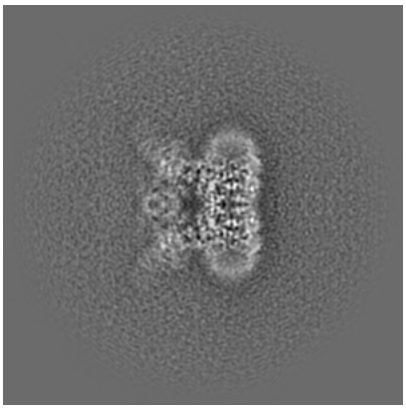
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

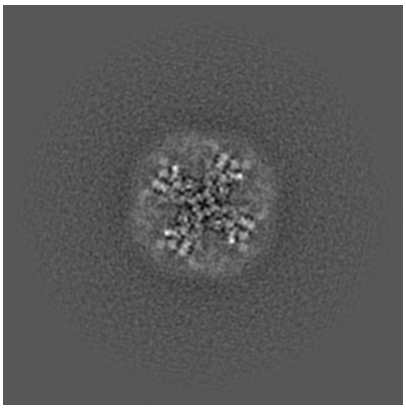
6.1.1 Primary map



X

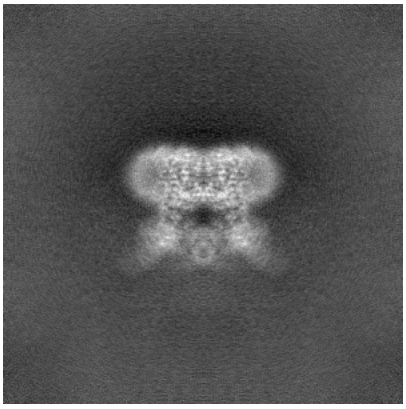


Y

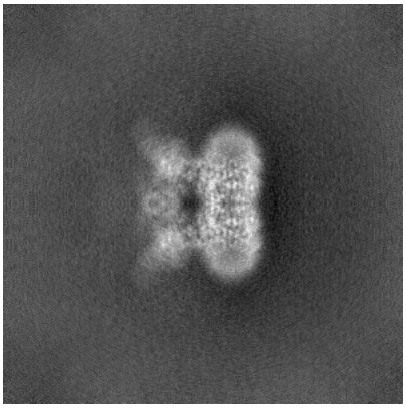


Z

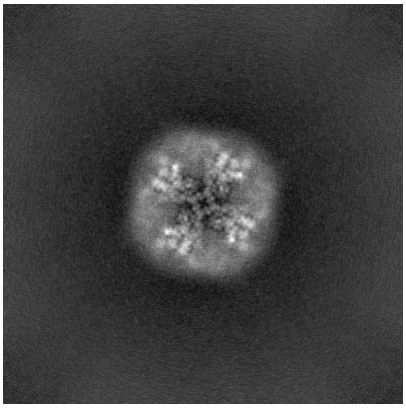
6.1.2 Raw map



X



Y

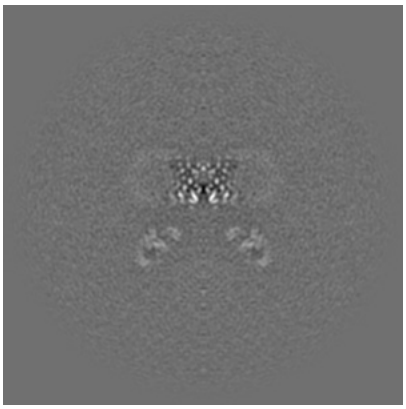


Z

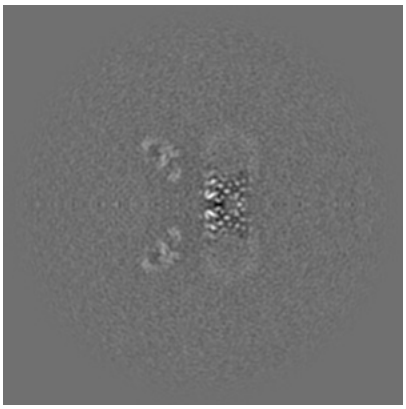
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

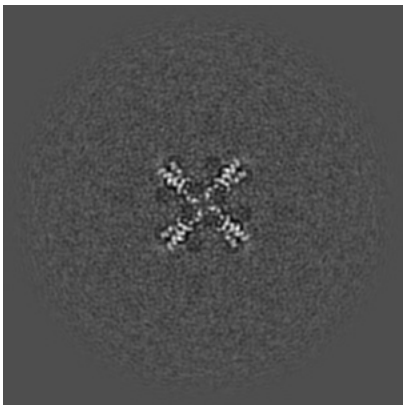
6.2.1 Primary map



X Index: 192

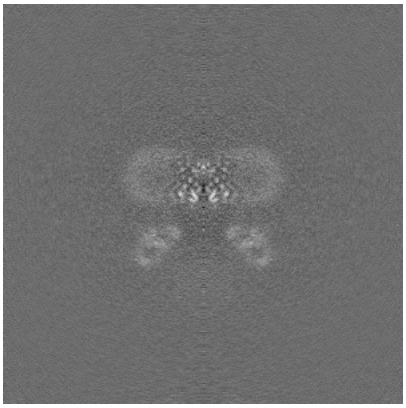


Y Index: 192

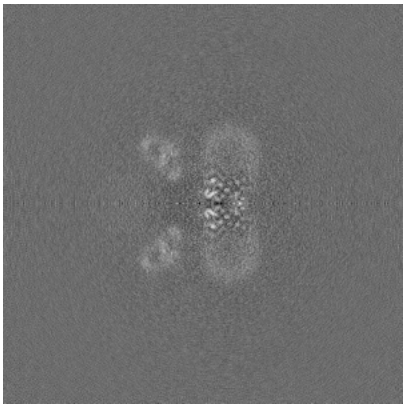


Z Index: 192

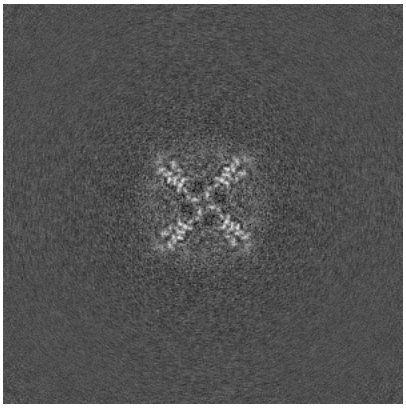
6.2.2 Raw map



X Index: 192



Y Index: 192

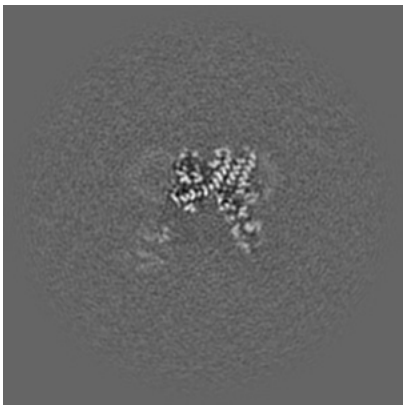


Z Index: 192

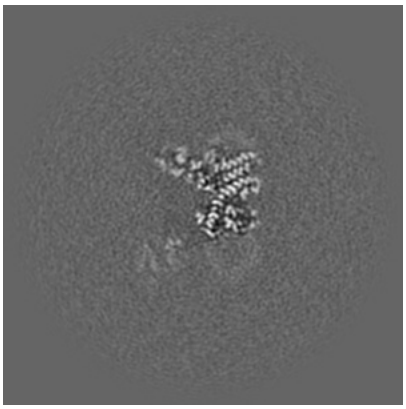
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

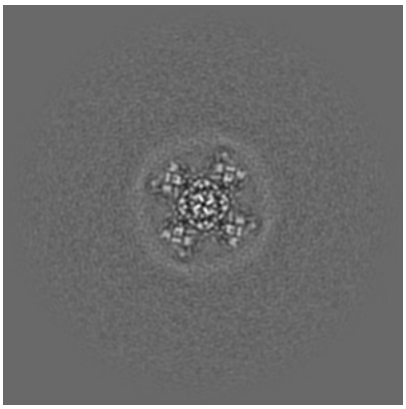
6.3.1 Primary map



X Index: 209

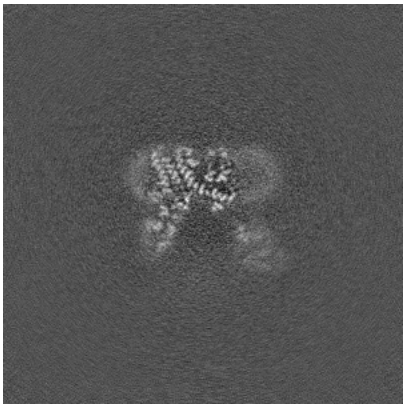


Y Index: 175

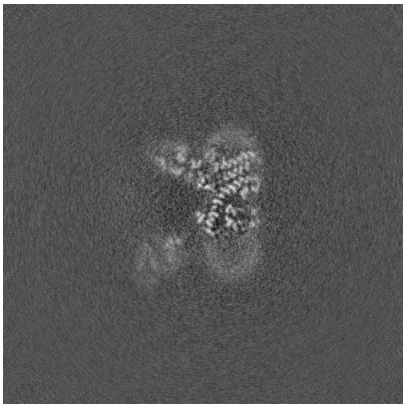


Z Index: 205

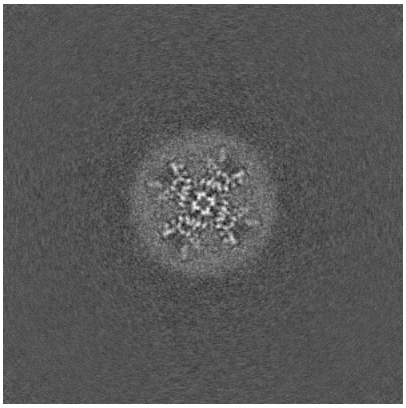
6.3.2 Raw map



X Index: 175



Y Index: 175

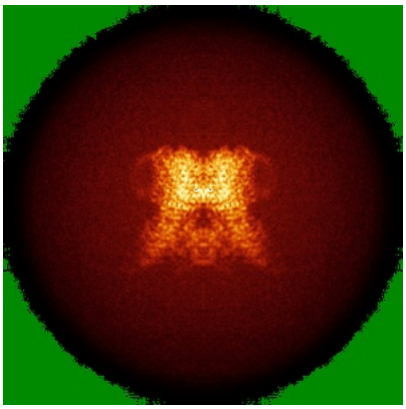


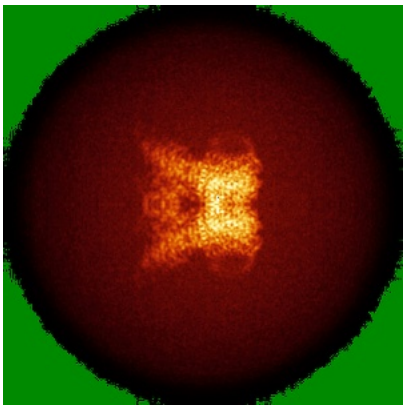
Z Index: 200

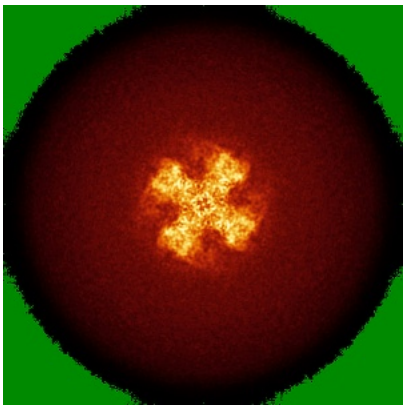
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

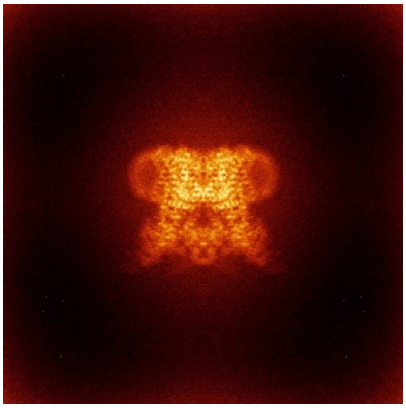
6.4.1 Primary map

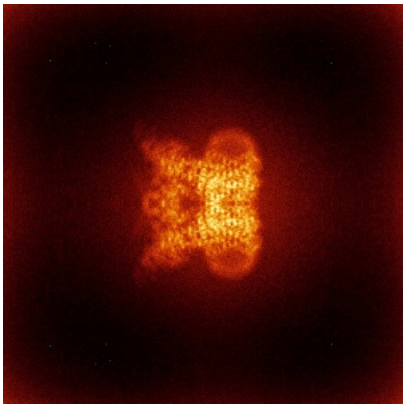

X

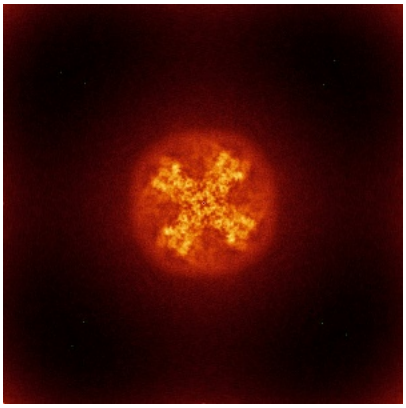

Y


Z

6.4.2 Raw map


X

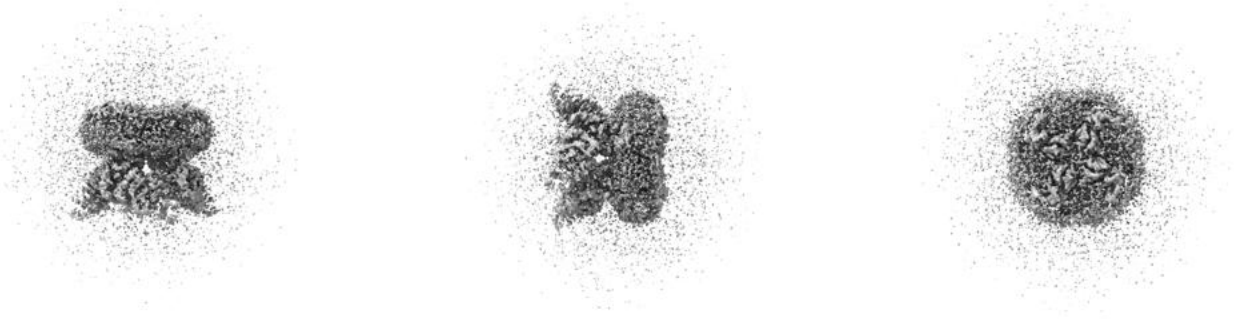

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

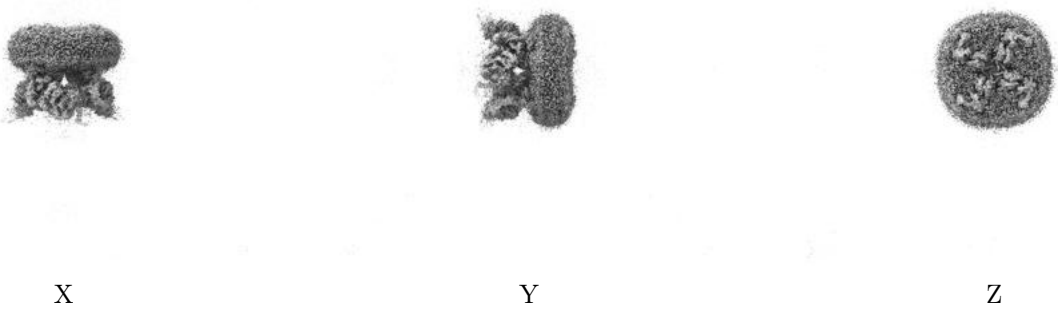
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

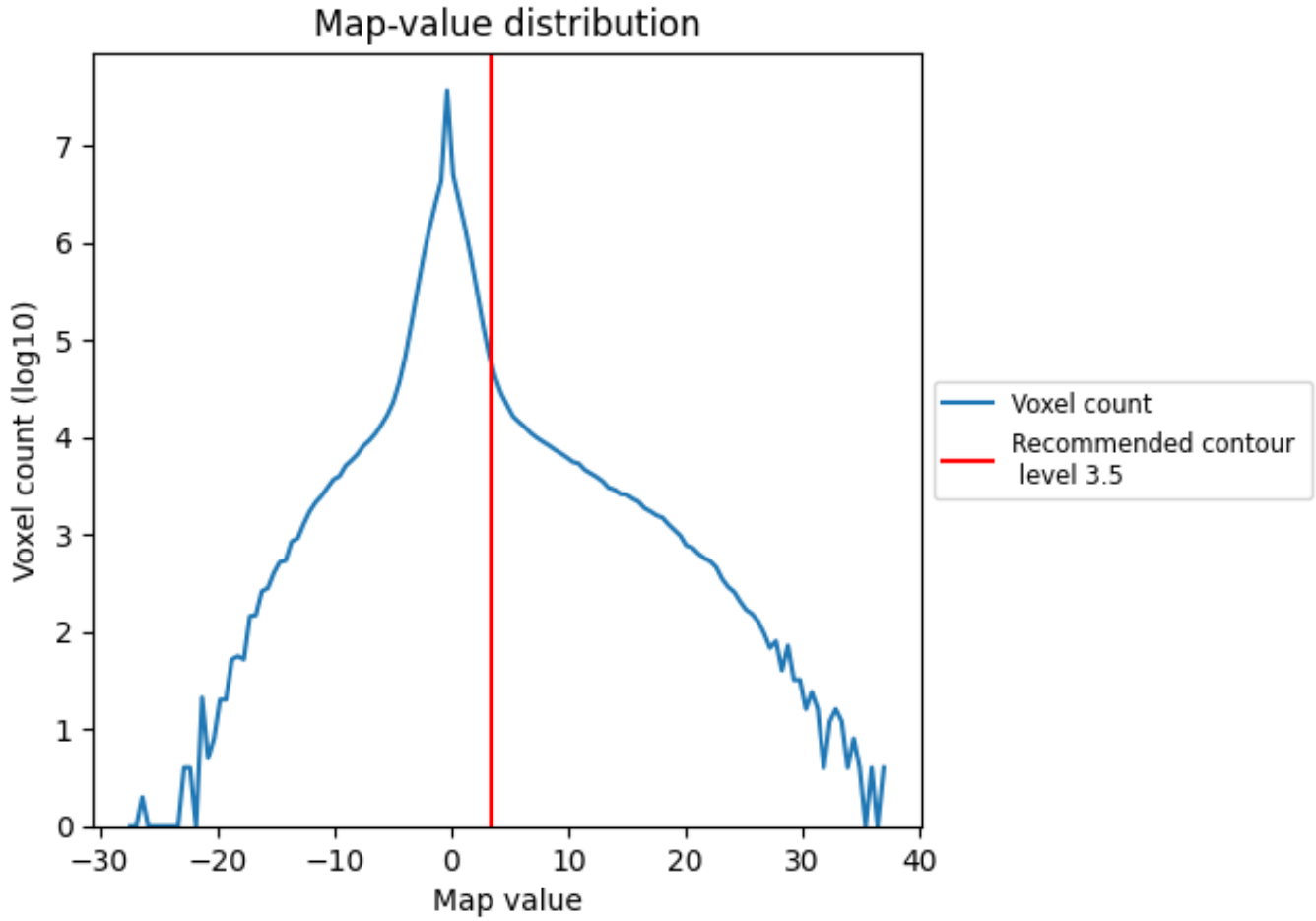
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

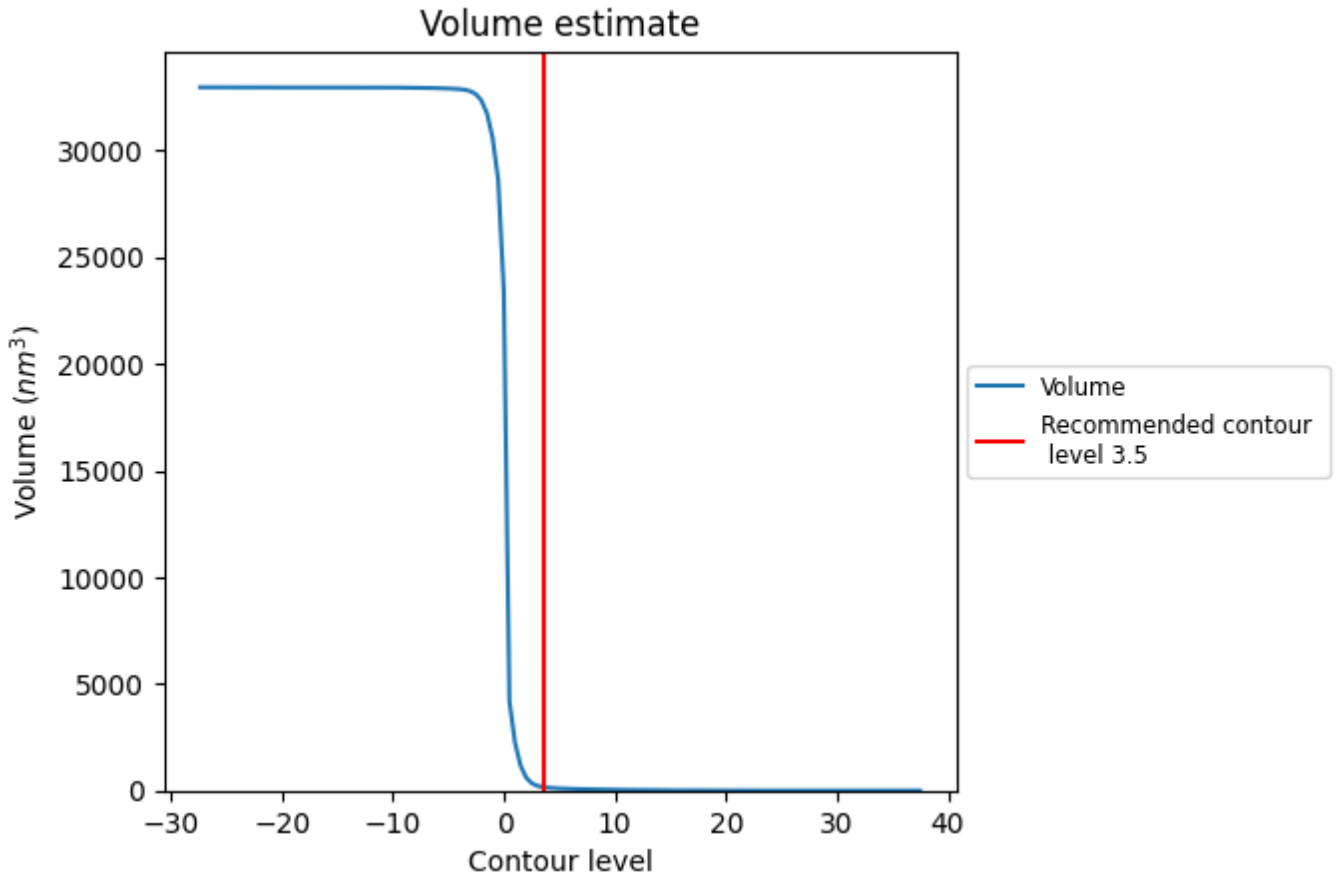
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

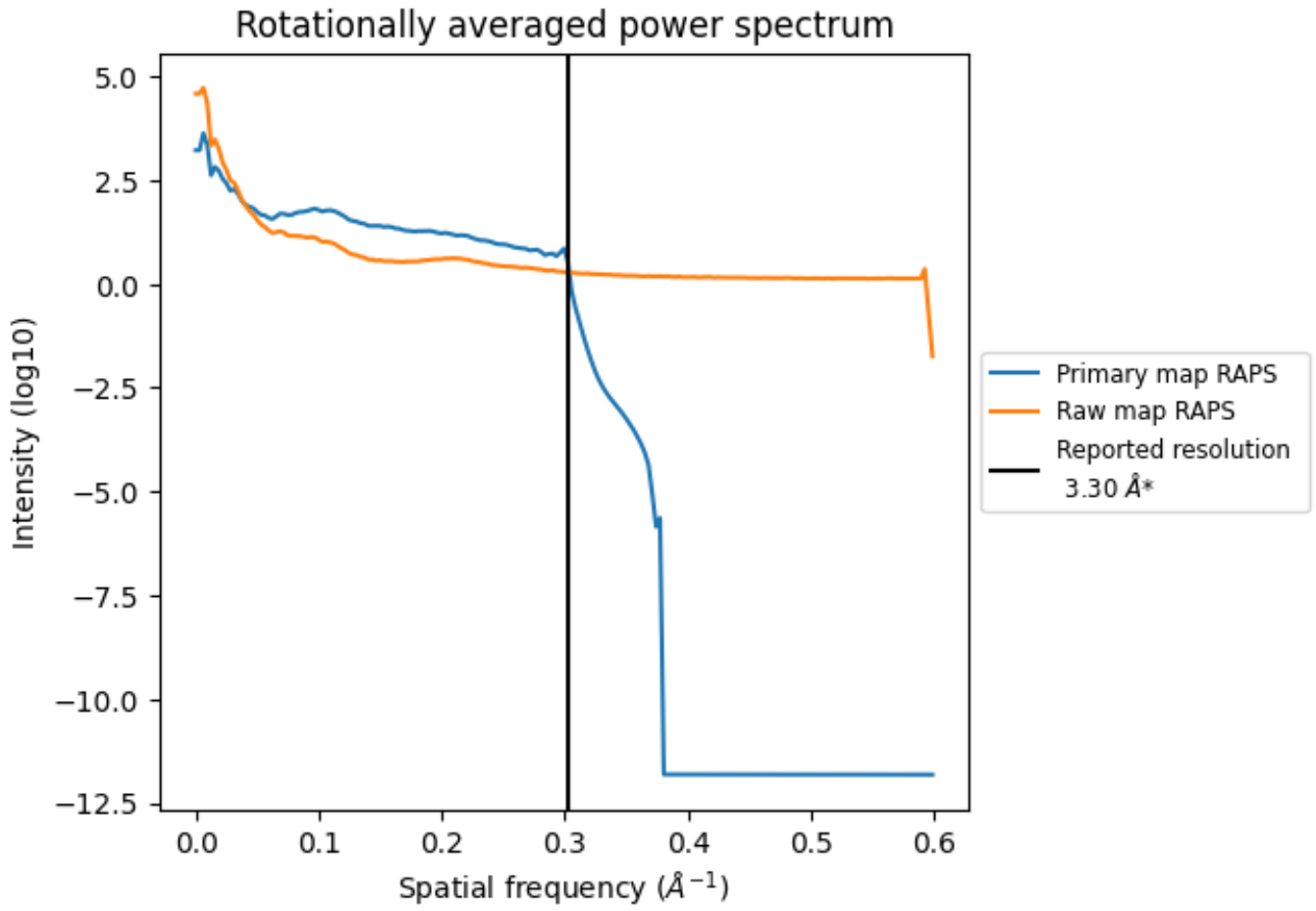
7.2 Volume estimate (i)



The volume at the recommended contour level is 165 nm^3; this corresponds to an approximate mass of 149 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

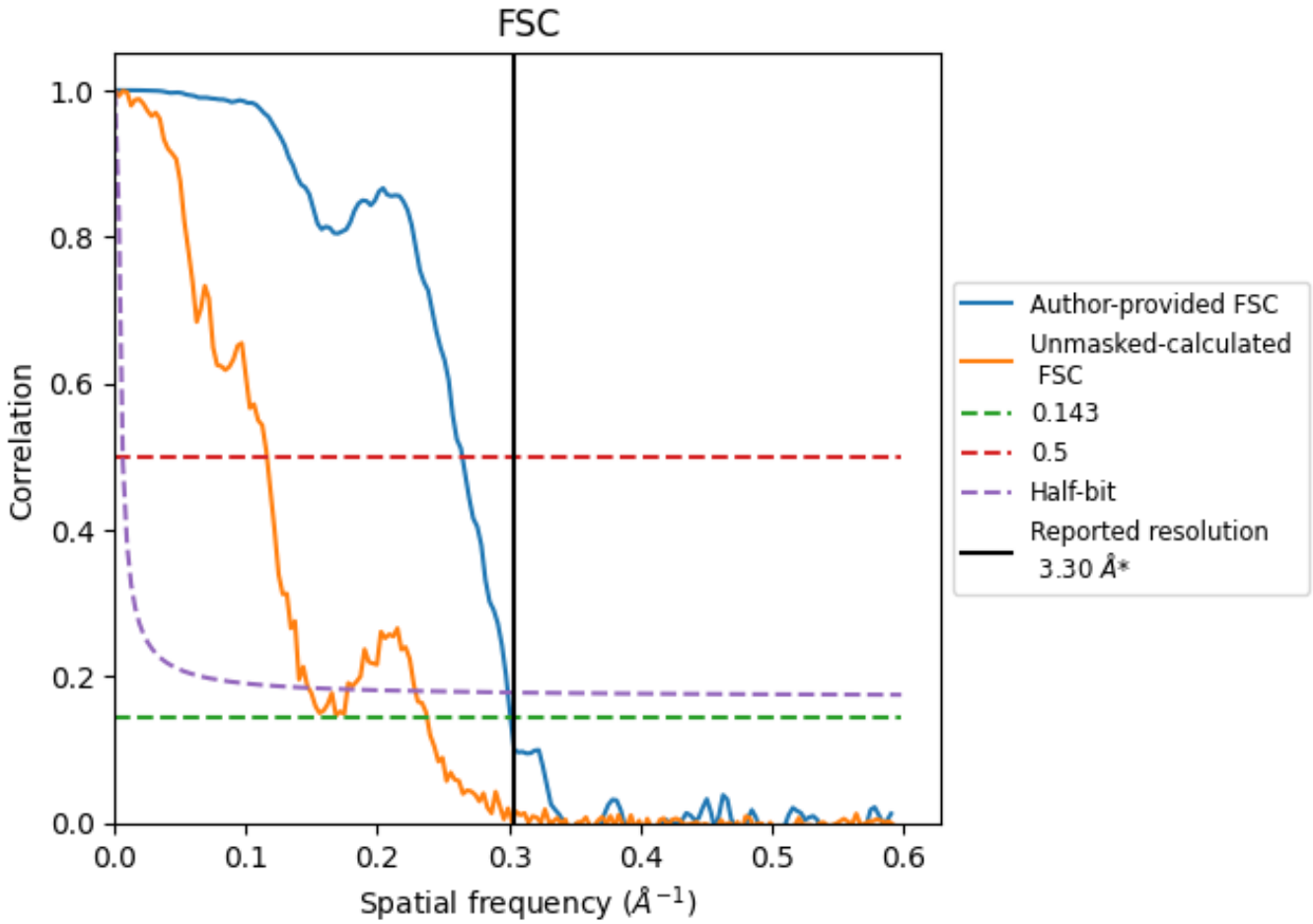


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8.2 Resolution estimates (i)

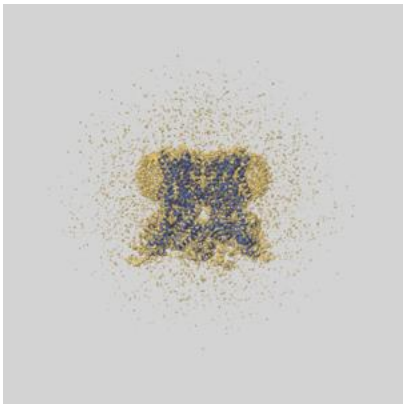
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.78	3.34
Unmasked-calculated*	4.21	8.64	6.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.3 by more than 10 %

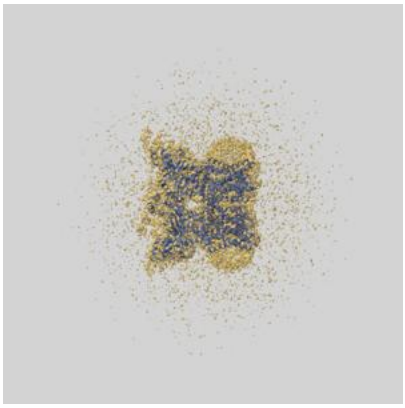
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40941 and PDB model 8T0E. Per-residue inclusion information can be found in section 3 on page 7.

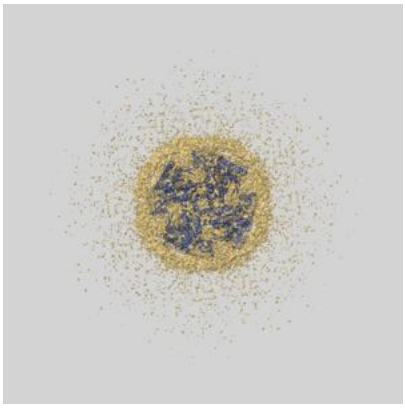
9.1 Map-model overlay



X



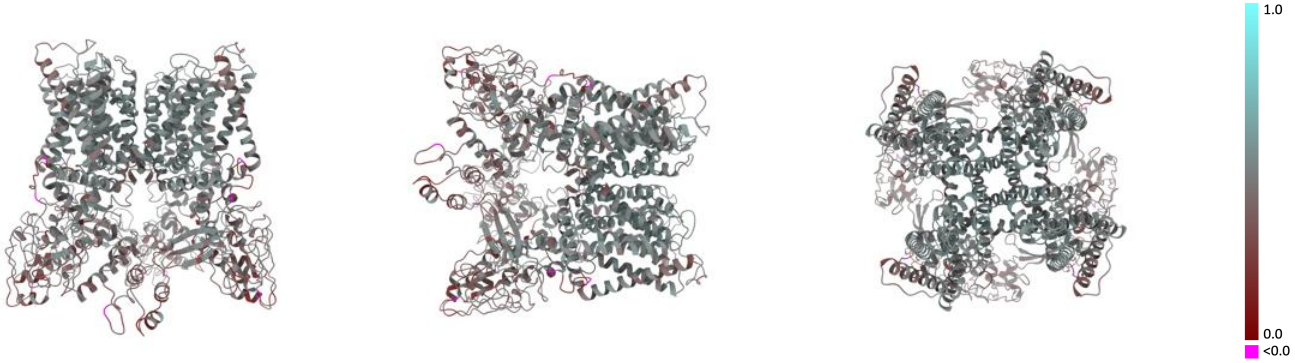
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

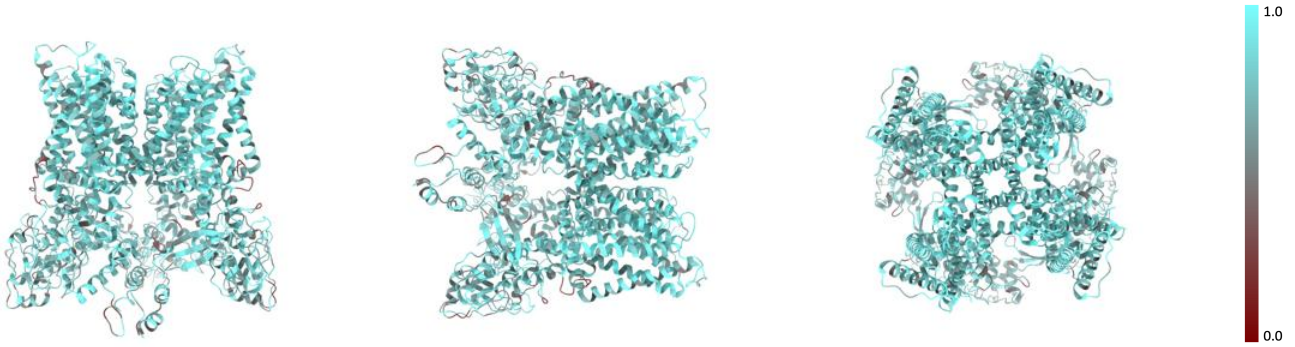
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

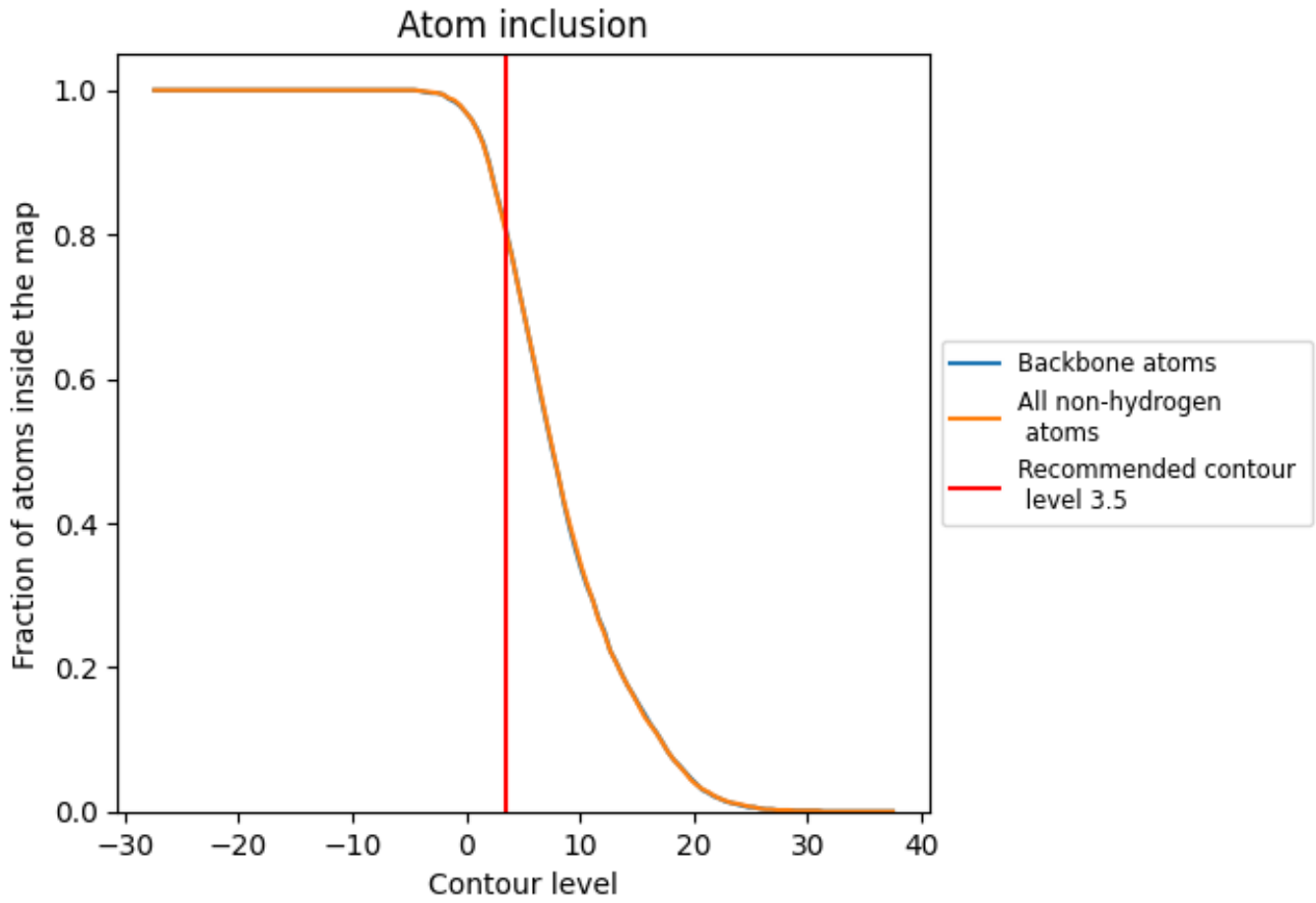
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.5).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.4620
A	0.8040	0.4620
B	0.8040	0.4620
C	0.8040	0.4610
D	0.8040	0.4610